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Applications of quadratic minimisation problems in statistics

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Albers et al. (2010) [2] showed that the problem $\min_{\mathbf{x}}(\mathbf{x}-\mathbf{t})'\mathbf{A}(\mathbf{x}-\mathbf{t})$ subject to $\mathbf{x}'\mathbf{B}\mathbf{x}+2\mathbf{b}'\mathbf{x} = k$ where $\mathbf{A}$ is positive definite or positive semi-definite has a unique computable solution. Here, several statistical applications of this problem are shown to generate special cases of the general problem that may all be handled within a general unifying methodology. These include non-trivial considerations that arise when (i) $\mathbf{A}$ and/or $\mathbf{B}$ are not of full rank and (ii) where $\mathbf{B}$ is indefinite. General canonical forms for $\mathbf{A}$ and $\mathbf{B}$ that underpin the minimisation methodology give insight into structure that informs understanding.

1. Introduction

Albers et al. [2] showed that the problem

$$\left.\begin{array}{l}\min\limits_{\mathbf{x}}(\mathbf{x}-\mathbf{t})'\mathbf{A}(\mathbf{x}-\mathbf{t})\\ \text{subject to } \mathbf{x}'\mathbf{B}\mathbf{x}+2\mathbf{b}'\mathbf{x}=k\end{array}\right\} \tag{1}$$

where $\mathbf{A}$ is positive definite or positive semi-definite, has a unique computable solution. The general approach adopted is to find a non-singular transformation $\mathbf{T}$ such that

$$\mathbf{T}'\mathbf{A}\mathbf{T}=\left(\begin{array}{cc|c}\mathbf{I} & & \\ & \mathbf{I} & \\ \hline & & \\ & & \end{array}\right);\qquad \mathbf{T}'\mathbf{B}\mathbf{T}=\left(\begin{array}{cc|cc}\Gamma_1 & & & \mathbf{D}_{10}\\ & \mathbf{0} & & \mathbf{D}_{00}\\ \hline & & \Gamma_0 & \\ \mathbf{D}_{10}' & \mathbf{D}_{00}' & & \mathbf{0}\end{array}\right). \tag{2}$$

The explicit form of $\mathbf{T}$ is given as Eq. (5) of Albers et al. [2].

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Eq. (2) is termed the General Canonical Form (GCF) of **A** and **B** and may be compared with classical canonical forms that arise when **B** is not indefinite. We may transform **x** and **t** to give $\mathbf{z} = \mathbf{T}^{-1}\mathbf{x} + \mathbf{m}$, $\mathbf{s} = \mathbf{T}^{-1}\mathbf{t} + \mathbf{m}$ for which (1) becomes

$$\left.\begin{array}{l}\min_{\mathbf{z}} \left(||\mathbf{z}_{11} - \mathbf{s}_{11}||^2 + ||\mathbf{z}_{10} - \mathbf{s}_{10}||^2\right) \\ \text{subject to :} \\ \begin{pmatrix}\mathbf{z}_{11}\\ \mathbf{z}_{10}\\ \mathbf{z}_{01}\\ \mathbf{z}_{00}\end{pmatrix}' \begin{pmatrix}\boldsymbol{\Gamma}_1 & & & \mathbf{D}_{10}\\ & \mathbf{0} & & \mathbf{D}_{00}\\ & & \boldsymbol{\Gamma}_0 & \\ \mathbf{D}_{10}' & \mathbf{D}_{00}' & & \mathbf{0}\end{pmatrix} \begin{pmatrix}\mathbf{z}_{11}\\ \mathbf{z}_{10}\\ \mathbf{z}_{01}\\ \mathbf{z}_{00}\end{pmatrix} + 2\begin{pmatrix}\mathbf{g}_{10}\\ \mathbf{g}_{00}\end{pmatrix}' \begin{pmatrix}\mathbf{z}_{10}\\ \mathbf{z}_{00}\end{pmatrix} = k\end{array}\right\}. \tag{3}$$

The definitions of all these matrices and vectors may be found in [2]. Suffice it to say here that they are easily calculable from spectral decompositions associated with **A** and **B** and the linear parameters **b**. $\boldsymbol{\Gamma}_1$ and $\boldsymbol{\Gamma}_0$ are diagonal matrices with no zero terms on the diagonals but at least one of them has negative elements when **B** is indefinite. The vector $\mathbf{z} = (\mathbf{z}_{11}', \mathbf{z}_{10}', \mathbf{z}_{01}', \mathbf{z}_{00}')$ is partitioned conformably with the partitions indicated in (3). The matrices $\mathbf{D}_{10}$ and $\mathbf{D}_{00}$ can only be present when **B** is indefinite and even then they are not always necessary. Thus, the quadratic form (3) is often diagonal, as in classical decompositions.

Having simplified (1)–(3), it turns out that the minimisation problem requires a unique solution λ_0 to the Fundamental Canonical Equation (FCE):

$$f(\lambda) = \mathbf{s}' (\mathbf{I} - \lambda\boldsymbol{\Gamma})^{-1} \boldsymbol{\Gamma} (\mathbf{I} - \lambda\boldsymbol{\Gamma})^{-1} \mathbf{s} = k \tag{4}$$

analogous to the characteristic equation in classical eigenvalue problems. Eq. (4) may be written as

$$f(\lambda) = \sum_{i=1}^{p} \frac{\gamma_i s_i^2}{(1 - \lambda\gamma_i)^2} = k \tag{5}$$

where, without loss of generality, k may be assumed non-negative.

The quantities γ_i, assumed to be arranged in non-decreasing order, arise as eigenvalues of a symmetric matrix derived from **A** and **B**. Eq. (5) usually has vertical asymptotes at $1/\gamma_i$ $(i = 1, \ldots, p)$ and may have many roots but λ_0 lies uniquely in an admissible region, containing the origin, bounded by $1/\gamma_1$ and $1/\gamma_p$, where the lower bound is replaced by $-\infty$ when γ_1 is non-negative. When zero s_1 and/or s_p occur, the asymptotes bounding the corresponding admissible region vanish (referred to as phantom asymptotes) and then λ_0 may be found in an enlarged region bounded by the first two asymptotes associated with non-zero values of s_i. A root λ^* will occur within this enlarged region. Then $\lambda_0 = \lambda^*$, $1/\gamma_1$, or $1/\gamma_p$ depending on whether λ^* is inside the admissible region or, if not, $f(0)$ is positive, or negative. Where there is no or only one non-phantom asymptote, then $\lambda_0 = 1/\gamma_1$ or $1/\gamma_p$.

2. Applications

In this section, we give some examples of where (1) is to be minimised. The solutions given are not necessarily the best or most up-to-date statistical treatments; they are chosen partly to show how the minimisation problem (1) can arise in a statistical context but also to illustrate how different variants, included in our general treatment, can arise.

Thus, in Sections 2.1 and 2.3 **A** and **B** are both p.s.d. and $t = \mathbf{0}$ while **s** may be distributed in different ways between the range and the null spaces of **A** and **B**. In Section 2.2 **B** is indefinite. In Section 2.4, the phantom asymptote problem can occur with, in the simplest cases, **B** p.d. but sometimes indefinite. In Section 2.5, **B** is indefinite but, because of a further simple linear constraint, may be transformed into p.s.d. form with a linear term **b**. And in Section 2.6, **B** is indefinite, $k = 0$ and **s** has zero components that induce the phantom asymptote effect.

We have tried to cover the major varieties of the problem, both from the statistical and algebraic points of view. Thus, in Section 2.1, we turn to reduced rank canonical variate analysis, in which both matrices are p.s.d. but without the vector **t** or the linear terms of (1). Sections 2.2 and 2.3 are concerned with mainstream statistical issues of quadratically constrained regression, possibly including linear constraints, and with spline fitting. Section 2.4 discusses two problems from Procrustes analysis, in the first of which (1) arises in a substantive way and in the second, in an algorithmic context. Section 2.5 discusses the Hardy–Weinberg estimation partly because it includes a linear term but also it has constraints additional to the quadratic in **B**. Finally, Section 2.6 gives an example of where **B** is indefinite and $k = 0$.

2.1. Canonical analysis

The problem of minimising the ratio of two quadratics

$$\rho = \frac{\mathbf{x}'\mathbf{A}\mathbf{x}}{\mathbf{x}'\mathbf{B}\mathbf{x}} \tag{6}$$

is common. When **A** and **B** are both p.d., the solution is well known to be given by the eigenvector associated with the minimal eigenvalue of the two-sided eigenvalue problem.

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{B}\mathbf{x},$$

the Lagrangian derived from minimising (6). The scaling of $\mathbf{x}$ is irrelevant but, for identification, something must be chosen and usually we choose $\mathbf{x}'\mathbf{B}\mathbf{x} = 1$. Then we can reformulate the problem in the form of (1) as minimising $\mathbf{x}'\mathbf{A}\mathbf{x}$ subject to the constraint $\mathbf{x}'\mathbf{B}\mathbf{x} = 1$.

Albers et al. [2] discussed (6), noting that in its most general form there is no interesting minimum (or maximum) of (6), it being possible to choose $\mathbf{x}$ so that the ratio is zero or infinity. Even when $\mathbf{A}$ and $\mathbf{B}$ are both p.s.d., the ratio may be made zero. The interesting and useful case is when $\mathbf{A}$ and $\mathbf{B}$ are both p.s.d. and the null space of one of them is contained in the null space of the other. This situation applies to several algebraically equivalent forms of canonical analysis in statistics: e.g. canonical variate analysis (CVA), canonical correlation analysis, optimal scores [9,15], multiple correspondence analysis/homogeneity analysis. The following discussion is set in the context of CVA but, with minor changes, applies to all such methods.

In CVA, the matrix $\mathbf{X}$ (assumed centred) is structured into K groups, supposed to be given in an indicator matrix $\mathbf{G}$ whose kth column gives membership of the kth group ($k = 1, 2, \ldots, K$). Then $\mathbf{X}'\mathbf{X} = \mathbf{T}^*$ is the total sums-of-squares-and-products matrix and the group means are given by $(\mathbf{G}'\mathbf{G})^{-1}\mathbf{G}'\mathbf{X}$ and the deviations from these means by $(\mathbf{I} - \mathbf{G}(\mathbf{G}'\mathbf{G})^{-1}\mathbf{G}')\mathbf{X}$. These contribute to the usual orthogonal between/within analysis of variance $\mathbf{T}^* = \mathbf{B}^* + \mathbf{W}$ as follows (we use $\mathbf{T}^*$ and $\mathbf{B}^*$ to distinguish the total and between groups dispersion matrices from the general matrices $\mathbf{T}$ and $\mathbf{B}$ occurring above)

$$\mathbf{X}'\mathbf{X} = \mathbf{X}'\mathbf{G}(\mathbf{G}'\mathbf{G})^{-1}\mathbf{G}'\mathbf{X} + \mathbf{X}'\left(\mathbf{I} - \mathbf{G}(\mathbf{G}'\mathbf{G})^{-1}\mathbf{G}'\right)\mathbf{X}. \tag{7}$$

Null vectors of $\mathbf{X}$ satisfy $\mathbf{X}\mathbf{v} = 0$. It follows from (7) that any null vector of $\mathbf{X}$ is also a null vector of $\mathbf{T}^*$, $\mathbf{B}^*$ and $\mathbf{W}$. Of course, $\mathbf{B}^*$ and $\mathbf{W}$ may have additional null vectors.

Because all matrices are p.s.d. we may simultaneously diagonalise any two of them (special case of (3)). Also, because all matrices share the null space of $\mathbf{T}^*$, then if we choose $\mathbf{T}^*$ to play the role of $\mathbf{A}$ in the GCF then, whichever plays the role of $\mathbf{B}$, the matrix $\boldsymbol{\Gamma}_0$ will vanish. Furthermore, because $\mathbf{T}^* = \mathbf{B}^* + \mathbf{W}$, having diagonalised $\mathbf{T}^*$ and $\mathbf{B}^*$, say, the same transformation must also diagonalise the third matrix $\mathbf{W}$. Taking all these things into account we have the following diagonalisations in the range space of $\mathbf{T}$.

$$\begin{aligned} &\mathbf{T}^* = \mathbf{B}^* + \mathbf{W} \\ &\begin{pmatrix} \mathbf{I} & & \\ & \mathbf{I} & \\ & & \mathbf{I} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\Gamma}_r & & \\ & \mathbf{I} & \\ & & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{I} - \boldsymbol{\Gamma}_r & & \\ & \mathbf{0} & \\ & & \mathbf{I} \end{pmatrix}. \end{aligned} \tag{8}$$

In (8) only the rows and columns associated with $\mathbf{z}_{11}$ and $\mathbf{z}_{10}$ of the GCF are represented, the remaining terms are zero, all being in the null space of $\mathbf{T}^*$. $\boldsymbol{\Gamma}_1$ is partitioned into two parts, $\boldsymbol{\Gamma}_r$ and $\mathbf{I}$, the latter being necessary to pair with the possible, but unlikely, occurrences of zero values in $\mathbf{W}$ other than those associated with the unshown null space shared with $\mathbf{T}^*$ and $\mathbf{B}^*$. Normally, $\mathbf{B}^*$ will have rank K, though it may be less, and normally $r = K$, but (8) allows for all possibilities. The matrices in (8) have been labelled $\mathbf{T}^*$, $\mathbf{B}^*$ and $\mathbf{W}$ though they are now in canonical form. Until further notice, we use these labels to refer to the canonical forms themselves.

Associate the vector $\mathbf{v}' = (\mathbf{v}_1', \mathbf{v}_2', \mathbf{v}_3')$ with the columns of the matrices in (8) then we have the quadratic forms:

$$(\mathbf{v}_1'\mathbf{v}_1 + \mathbf{v}_2'\mathbf{v}_2 + \mathbf{v}_3'\mathbf{v}_3) = (\mathbf{v}_1'\boldsymbol{\Gamma}_r\mathbf{v}_1 + \mathbf{v}_2'\mathbf{v}_2) + (\mathbf{v}_1(\mathbf{I} - \boldsymbol{\Gamma}_r)\mathbf{v}_1 + \mathbf{v}_3'\mathbf{v}_3). \tag{9}$$

To minimise $\mathbf{v}'\mathbf{W}\mathbf{v}$, we merely have to choose $\mathbf{v} = (\mathbf{0}, \mathbf{v}_2, \mathbf{0})$ giving, $\mathbf{v}'\mathbf{T}^*\mathbf{v} = \mathbf{v}'\mathbf{B}^*\mathbf{v} = \mathbf{v}_2'\mathbf{v}_2$, $\mathbf{v}'\mathbf{W}\mathbf{v} = 0$. Thus we have an absolute minimum whichever of $\mathbf{v}'\mathbf{T}^*\mathbf{v}$ and $\mathbf{v}'\mathbf{B}^*\mathbf{v}$ may be used as a denominator and whatever normalisation may be used. If $\mathbf{W}$ has a zero term in (8), nothing better can be done. A zero term implies zero deviation from the group means in all groups and is an uninteresting case, the corresponding canonical variables being discarded in the same way as the variables in the null space of $\mathbf{T}^*$. Usually, $\mathbf{W}$ will not have this zero term and then (9) simplifies to

$$(\mathbf{v}_1'\mathbf{v}_1 + \mathbf{v}_3'\mathbf{v}_3) = (\mathbf{v}_1'\boldsymbol{\Gamma}_r\mathbf{v}_1) + (\mathbf{v}_1(\mathbf{I} - \boldsymbol{\Gamma}_r)\mathbf{v}_1 + \mathbf{v}_3'\mathbf{v}_3).$$

Now, minimising $\mathbf{v}'\mathbf{W}\mathbf{v}$ relative to either $\mathbf{v}'\mathbf{T}^*\mathbf{v}$ or $\mathbf{v}'\mathbf{B}^*\mathbf{v}$ is equivalent to requiring the maximisation of

$$\frac{\mathbf{v}_1'\boldsymbol{\Gamma}_r\mathbf{v}_1}{\mathbf{v}_1'\mathbf{v}_1 + \mathbf{v}_3'\mathbf{v}_3}. \tag{10}$$

Whatever the value of $\mathbf{v}_1$ in (10), the ratio is always greatest when $\mathbf{v}_3 = 0$, the maximum $\gamma_{\max}$ occurring when $\mathbf{v}_1$ is zero except for the position corresponding to $\gamma_{\max}$. In the current context, the transformation $\mathbf{x} = \mathbf{T}^{-1}\mathbf{v}$ (see (5) in [2]) between the canonical variables $\mathbf{v}$ and the original variables $\mathbf{x}$ is greatly simplified.

Krzanowski et al. [17] consider the analysis of spectroscopic data where $\mathbf{X}$ has n (30–200) rows representing samples and p (200–4000) columns representing frequencies, treated as variables. With data like these the ranks of $\mathbf{T}^*$, $\mathbf{B}^*$, and $\mathbf{W}$ will be much less than the order of the matrices p. The above justifies what Krzanowski et al. [17] term the PPC method and other methods they describe where $\mathbf{W}$ is modified to reduce the effects of dimensions in which variation, if not actually zero, is deemed to be sufficiently small to be ignored (see also [20]).

Eq. (8) is particularly simple. This is a consequence of the between and within groups formulation and it should not be thought that these results extend to general ratios of p.s.d. quadratic forms. Newcomb [21] is usually regarded as the first to discuss the simultaneous diagonalisation of two symmetric semi-definite matrices. See [28] for a survey. Conditions under which (6) has an acceptable optima for general p.s.d. matrices $\mathbf{B}$ and $\mathbf{W}$ are discussed by Rao and Mitra [22], McDonald et al. [19] and De Leeuw [8] where the effects of the matrix $\boldsymbol{\Gamma}_0$ must also be considered.

CVA usually uses two or more eigenvectors from the solution to (6). In so doing, one is prepared to accept a "second best vector that is orthogonal to the first" but such solutions are no longer solutions to our problem (1). Note that although (6), even in reduced rank forms, does not depend on the scaling of $\mathbf{x}$, once we choose two or more vectors, their relative scaling becomes critical. Further formulating the problem in Lagrangian form brings into question the precise nature of the constraints adopted (see e.g. [16,10]). The full details of these problems go beyond the limits of this paper, and is presented in [11,3].

2.2. Normal linear models with quadratic constraints

Multiple regression problems, where the regression coefficients are subject to some constraints are common. Thus, we require to solve

$$\left.\begin{array}{l}\min\limits_{\boldsymbol{\beta}}(\mathbf{y}-\mathbf{X}\boldsymbol{\beta})'(\mathbf{y}-\mathbf{X}\boldsymbol{\beta})\\ \text{subject to } g(\boldsymbol{\beta})=0\end{array}\right\}.$$

If $\mathbf{b}_0$ is the OLS estimator of $\boldsymbol{\beta}$ we could do the minimisation as

$$\left.\begin{array}{l}\min((\mathbf{y}-\mathbf{X}\mathbf{b}_0)+(\mathbf{X}\mathbf{b}_0-\mathbf{X}\boldsymbol{\beta}))'((\mathbf{y}-\mathbf{X}\mathbf{b}_0)+(\mathbf{X}\mathbf{b}_0-\mathbf{X}\boldsymbol{\beta}))\\ \text{subject to } g(\boldsymbol{\beta})=0\end{array}\right\}$$

which, because of the orthogonality of $\mathbf{X}$ and $(\mathbf{y}-\mathbf{X}\mathbf{b}_0)$ simplifies to

$$\left.\begin{array}{l}\min((\mathbf{y}-\mathbf{X}\mathbf{b}_0)'(\mathbf{y}-\mathbf{X}\mathbf{b}_0)+(\boldsymbol{\beta}-\mathbf{b}_0)'\mathbf{X}'\mathbf{X}(\boldsymbol{\beta}-\mathbf{b}_0))\\ \text{subject to } g(\boldsymbol{\beta})=0\end{array}\right\}.$$

Thus, because the first term of the preceding objective function does not depend on $\boldsymbol{\beta}$ we require to solve

$$\left.\begin{array}{l}\min(\mathbf{b}_0-\boldsymbol{\beta})'\mathbf{X}'\mathbf{X}(\mathbf{b}_0-\boldsymbol{\beta})\\ \text{subject to } g(\boldsymbol{\beta})=0\end{array}\right\}$$

showing that the constrained solution (whatever the constraint) is given by the nearest constrained point (in the metric $\mathbf{X}'\mathbf{X}$) to the unconstrained solution. When $g(\boldsymbol{\beta})=0$ is a quadratic constraint, this problem is manifestly in the form of (1) where $\mathbf{A}=\mathbf{X}'\mathbf{X}$ and $\mathbf{t}=\mathbf{b}_0$.

In the above, we have implicitly assumed that $\mathbf{b}_0$ is unique. However, when $\mathbf{X}$ is not of full column-rank, if $\mathbf{b}_0$ is one solution, then so is $\mathbf{b}_0+\mathbf{c}$, where $\mathbf{c}$ is any vector in the null space of $\mathbf{X}$. This arbitrary vector has no effect on the value of the minimum but does determine a range of equally valid solutions that satisfy the constraint. This is a general property, described in detail by Albers et al. [2] when $\mathbf{t}$ contains components in the null space of $\mathbf{A}$ that are in the range space of $\mathbf{B}$ and may be handled by our general approach.

As an explicit example, consider the following normal linear model $\mathbf{y}=\mathbf{X}\boldsymbol{\beta}+\boldsymbol{\varepsilon}$ where $\boldsymbol{\beta}'=(\beta_0,\beta_1,\beta_2)$ is a vector comprising the intercept and two non-zero slopes, $\mathbf{X}=(\mathbf{1},\mathbf{x}_1,\mathbf{x}_2)$ consists of a column of ones and two columns of exogenous variables, and $\boldsymbol{\varepsilon}$ is a vector of i.i.d. $\mathcal{N}(0,\sigma^2)$ residuals.

Gregory and Veall [14] were interested in whether $\beta_1\beta_2=1$, so considered testing (a) $\mathrm{H}_0^a: g^a(\boldsymbol{\beta})=\beta_1-1/\beta_2=0$ or, algebraically equivalent, (b) $\mathrm{H}_0^b: g^b(\boldsymbol{\beta})=\beta_1\beta_2-1=0$. It is immediately clear that H_0^b can be written in the quadratic form $\boldsymbol{\beta}'\mathbf{B}\boldsymbol{\beta}$ with $\mathbf{B}$ a zero matrix, except for $(\mathbf{B})_{23}=1/2$; hence this example is of the form of (1).

Both hypotheses were studied because each yields a different Wald statistic

$$W=g(\hat{\boldsymbol{\beta}})'\left(\left(\frac{\partial g(\hat{\boldsymbol{\beta}})}{\partial\boldsymbol{\beta}}\right)I(\hat{\boldsymbol{\beta}})^{-1}\left(\frac{\partial g(\hat{\boldsymbol{\beta}})}{\partial\boldsymbol{\beta}}\right)'\right)^{-1}g(\hat{\boldsymbol{\beta}}),$$

where I represents the Fisher information matrix, due to the nonlinear relationship under investigation (cf. [18]). Critchley et al. [7] explain the difference in behaviour via differential geometry. They outline a general approach to minimum distance estimation based on the Fisher geodesic statistic, obtained by computing the squared distance between $\hat{\boldsymbol{\beta}}$ and the constraint using the Fisher information matrix as the metric tensor. In the special case of the normal linear model, the resulting methodology takes the form of (1).

2.3. Smoothing by splines with bounded roughness

Splines can be used to construct an estimate of a smooth (i.e. twice differentiable) curve for which a number of values $x_1,\ldots,x_n$ $(n>3)$ have been observed at locations $t_1<t_2<\cdots<t_n$ in (a,b). Splines need to fulfil two contradictory tasks:

(i) to fit the data as well as possible and (ii) to be as smooth as possible. Reinsch [23] introduced the following approach, which fits into our methodology. His splines $g(\cdot)$ are the solution to the following optimisation problem

$$\min_g \sum_{i=1}^{n} (x_i - g(t_i))^2 \quad \text{subject to} \int_a^b \left(g''(x)\right)^2 \, dx \le k, \tag{11}$$

i.e. the goodness-of-fit is measured by the residual sum-of-squares, and the smoothness by the integral of the squared second derivative. Changing the inequality sign of (11) to an equality sign does not affect the solution(s).

It can be shown that the optimal $\hat{g}$ has the form of a natural cubic spline (NCS) (see, e.g., [13]). Without going into too much detail, a function $g(\cdot)$ is called a NCS if (i) on each interval (t_i, t_{i+1}), g is a cubic polynomial, (ii) $\lim_{t\uparrow t_i} g(t) = \lim_{t\downarrow t_i} g(t)\ \forall i$, similar properties holding for g' and g'', and (iii) some regularity conditions hold for $g(t_1)$ and $g(t_n)$. It is possible to completely specify a NCS by two vectors, $\mathbf{g}$ with $g_i = g(t_i)$ and $\boldsymbol{\gamma}$ with $\gamma_i = g''(t_i)$. From the positions t_i we define matrices $\mathbf{Q}(n \times (n-2))$ and $\mathbf{R}$ $((n-2) \times (n-2))$ via

$$(\mathbf{Q})_{ij} = \begin{cases} \left(t_j - t_{j-1}\right)^{-1} & i = j-1 \\ -\left(t_j - t_{j-1}\right)^{-1} - \left(t_{j+1} - t_j\right)^{-1} & i = j \\ \left(t_{j+1} - t_j\right)^{-1} & i = j+1 \\ 0 & |i-j| > 1 \end{cases}$$

for $j = 2, \ldots, n-1$ and

$$(\mathbf{R})_{ij} = \begin{cases} \frac{1}{3}\left(\left(t_j - t_{j-1}\right)^{-1} + \left(t_{j+1} - t_j\right)^{-1}\right) & i = j \\ \frac{1}{6}\left(t_{j+1} - t_j\right)^{-1} & i = j \pm 1 \\ 0 & |i-j| > 1 \end{cases}$$

for $j = 2, \ldots, n-1$. From $\mathbf{Q}$ and $\mathbf{R}$ we obtain $\mathbf{K}$ via $\mathbf{K} = \mathbf{Q}\mathbf{R}^{-1}\mathbf{Q}'$. Now (11) can be rewritten in the form (1) as

$$\left.\begin{array}{l} \min_{\mathbf{g}} (\mathbf{x} - \mathbf{g})'(\mathbf{x} - \mathbf{g}) \\ \text{subject to } \mathbf{g}'\mathbf{K}\mathbf{g} \le k \end{array}\right\}. \tag{12}$$

Nowadays a slightly different optimisation problem,

$$\min_{\mathbf{g}} \left((\mathbf{x} - \mathbf{g})'(\mathbf{x} - \mathbf{g}) + \alpha \mathbf{g}'\mathbf{K}\mathbf{g}\right) \tag{13}$$

for some $\alpha \ge 0$, is often used (cf. [13]). This problem has an explicit solution for a given α, but in general the choice of α will be data dependent and decided via e.g. cross validation, resulting in a methodology outside the scope of (1).

2.4. *Problems in Procrustes analysis*

2.4.1. *Oblique axes*

The origins of Procrustes analysis in psychometrics are concerned with transformations to oblique axes. The simplest problem of this kind is to minimise

$$||\mathbf{X}\mathbf{C} - \mathbf{Y}||^2$$

where $\mathbf{X}$ gives one set of coordinates and $\mathbf{Y}$ another set (termed the target) and direction cosines $\mathbf{C}$ of oblique axes are sought to give the best match. Thus $\mathbf{C}$ is a direction cosine matrix and therefore has columns with unit sum-of-squares. It is clear that the optimisation can be done column by column, so that it is only necessary to solve the problem (14),

$$\min_{\mathbf{c}} ||\mathbf{X}\mathbf{c} - \mathbf{y}||^2 \quad \text{subject to } \mathbf{c}'\mathbf{c} = 1 \tag{14}$$

which is in the form of one of a simple reparameterisation of (1), so our methods are immediately applicable. A full solution to minimising (14) was given by Browne [5] using methods that are antecedents to those described in [2]. It was in this context that Cramer [6] first recognised the potential problem of what we term phantom asymptotes and proposed methods subsequently improved by Ten Berge and Nevels [27].

Gower and Dijksterhuis [12, Chapter 6] discuss oblique axes variants in which $\mathbf{C}$ is replaced by $\mathbf{C}'$, $\mathbf{C}^{-1}$ or $(\mathbf{C}')^{-1}$ and in which the constraint need not be positive definite but the GCF remains diagonal. In these variants the columns of $\mathbf{C}$ cannot be estimated independently so our methods have to be used iteratively.

2.4.2. Missing values

The generalised Procrustes problem is

$$\min_{\mathbf{T}_k} \sum_{k=1}^{K} ||\mathbf{X}_k\mathbf{T}_k - \mathbf{G}||^2 \quad \text{where } \mathbf{G} = \frac{1}{K}\sum_{k=1}^{K}\mathbf{X}_k\mathbf{T}_k \tag{15}$$

where $\mathbf{T}_k$ is constrained to belong to some matrix class, typically orthogonal. It may be assumed that each $\mathbf{X}_k$ is column centred, $\mathbf{1}'\mathbf{X}_k = 0$. We shall need an alternative, but equivalent, form of (15)

$$\min_{\mathbf{T}_k} \left(\frac{K-1}{K}\right)^2 \sum_{k=1}^{K} ||\mathbf{X}_k\mathbf{T}_k - \mathbf{G}_k||^2 \quad \text{where } \mathbf{G}_k = \frac{1}{K-1}\sum_{i\neq k}^{K}\mathbf{X}_i\mathbf{T}_i. \tag{16}$$

$\mathbf{G}$ is termed the group average and $\mathbf{G}_k$ the k-excluded group average. We assume that a method is available for minimising (15) and (16) but suppose $\mathbf{X}_k$ ($k = 1, 2, \dots, K$) has missing values. Because the k-excluded group average does not depend on $\mathbf{X}_k$, the missing values for each $\mathbf{X}_k$ may be estimated independently. We assume an iterative process with current estimates of the missing values and seek to find an updating matrix $\mathbf{X}$ that is zero except for values, to be calculated, in positions corresponding to the values missing in the kth set. The update should preserve the centring property, so we wish to find $\mathbf{X}$ satisfying

$$\min_{\mathbf{X}} ||(\mathbf{I}-\mathbf{N})(\mathbf{X}_k - \mathbf{X})\mathbf{T}_k - \mathbf{G}_k||^2 \tag{17}$$

where $\mathbf{N}$ is the matrix $\mathbf{11}'/n$. An additional requirement is that the size of $\mathbf{X}_k$ should be the same before and after updating. Thus

$$\operatorname{trace}(\mathbf{X}_k - \mathbf{X})'(\mathbf{I}-\mathbf{N})(\mathbf{X}_k - \mathbf{X}) = \operatorname{trace}(\mathbf{X}_k'\mathbf{X}). \tag{18}$$

Clearly, both the objective function (17) and the constraint (18) are quadratic in the elements of $\mathbf{X}$, so we have a problem of our basic type (1). We do not give the detailed manipulations to get these forms to coincide with (1) but a first step is to define $\mathbf{x} = \operatorname{vec}(\mathbf{X})$ and $\mathbf{x}_k = \operatorname{vec}(\mathbf{X}_k)$ and then express the quadratic functions as functions of $\mathbf{x}$. Ten Berge et al. [26] made an initial study of this problem and Gower and Dijksterhuis [12] give further details that fully cover the centring requirement but handle the size constraint by ad hoc methods; the rather heavy, but basically straightforward, algebra required for the full solution is reported elsewhere [4].

We note that if this method were to be used when $\mathbf{T}_k = \mathbf{C}_k$, an oblique axis direction cosine matrix, then (1) arises both in the estimation of $\mathbf{C}_k$ and in the estimation of the missing values.

2.5. Hardy–Weinberg equilibrium

In genetics, we may have three genotypes denoted by AA, BB, AB occurring in proportions $\mathbf{p} = (p_1, p_2, p_3)$. Under random mating, these proportions remain unchanged when the Hardy–Weinberg equilibrium condition is satisfied.

$$p_3^2 = 4p_1p_2. \tag{19}$$

When proportions $\mathbf{q} = (q_1, q_2, q_3)$ are observed, we may wish to estimate $\mathbf{p}$. Maximum likelihood estimation based on a multinomial distribution might be used (see below) but first we examine least-squares estimation.

$$\min_{\mathbf{p}} ||\mathbf{p}-\mathbf{q}||^2 \quad \text{subject to } p_3^2 = 4p_1p_2, \tag{20}$$

which is in the form of Eq. (1), so the results described in the Introduction would be immediately available were it not for the need to accommodate the additional constraints $\mathbf{1}'\mathbf{p} = 1$ and $\mathbf{p} \geq 0$. Before showing how to do this, we note that for fixed p_3, (19) represents a rectangular hyperbola in the plane of p_1, p_2, so the surface described by the constraint is a series of increasingly large rectangular hyperbolae as one moves away from the origin in the direction of p_3 and so the constraint is indefinite.

The additional constraint $\mathbf{1}'\mathbf{p} = 1$ can be handled by transforming into coordinates $\mathbf{z}$ in the plane $\mathbf{1}'\mathbf{p} = 1$. Thus $\mathbf{z} = \mathbf{Hp}$ where $\mathbf{H}$ is the orthogonal matrix,

$$\mathbf{H} = \begin{pmatrix} \frac{1}{\sqrt{2}} & & \\ & \frac{1}{\sqrt{6}} & \\ & & \frac{1}{\sqrt{3}} \end{pmatrix} \begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & -2 \\ 1 & 1 & 1 \end{pmatrix}$$

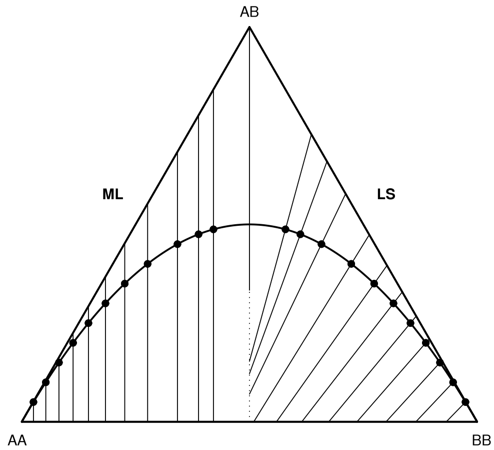

Fig. 1. Contours of same equilibrium prediction. Left-hand side: maximum likelihood contours, perpendicular to base line. Right-hand side: least-squares contours, normal to the equilibrium parabola.

the diagonal matrix giving the normalisers. With this change of axes we find that the constraint becomes

$$z_2^2 = \frac{\sqrt{6}}{3} z_1 + \frac{1}{6} \tag{21}$$

which represents a parabola in the plane $\mathbf{1}'\mathbf{p} = 1$, termed the equilibrium parabola. We find it interesting that this slice through the rectangular hyperbolic structure described above is parabolic and so we are no longer concerned with an indefinite constraint. Next, consider the effect of the transformation on the objective function. We have

$$||\mathbf{p} - \mathbf{q}||^2 = (\mathbf{p} - \mathbf{q})'(\mathbf{p} - \mathbf{q}) = (\mathbf{p} - \mathbf{q})'\mathbf{H}'\mathbf{H}(\mathbf{p} - \mathbf{q}) = (\mathbf{z} - \mathbf{r})'(\mathbf{z} - \mathbf{r})$$

where $\mathbf{r} = \mathbf{Hq}$. Now, because $\mathbf{p}$ and $\mathbf{q}$ are proportions then $z_3 = r_3 = 1/\sqrt{3}$ and the final term vanishes, giving the transformed version of the objective function

$$(z_1 - r_1)^2 + (z_2 - r_2)^2. \tag{22}$$

Thus, the problem is transformed into minimising (22) subject to (21). This is in the form of (1) while ensuring that the constraint $\mathbf{1}'\mathbf{p} = 1$ is satisfied. Furthermore, (21) is in the GCF (with z_1 as linear variable), which was not so for (20). Thus, provided $\mathbf{q}$ satisfies these constraints (see below), it follows that the minimisation of (22) automatically delivers a result that also satisfies the constraints including a non-extraneous linear term. Thus, the problem is now in the GCF form described in Section 1 and may be solved by a standard algorithm designed for the general case.

Contours of equal least-squares estimates, being shortest distances, must be normal to the equilibrium parabola, as shown on the right-hand side of Fig. 1. This diagram confirms that so long as $\mathbf{q}$ is within the triangle, then so is its estimate $\mathbf{p}$, so guaranteeing that $\mathbf{p} \geq 0$ as well as $\mathbf{1}'\mathbf{p} = 1$.

For comparison, the multinomial maximum likelihood estimates are

$$p_1 = q_1 + a, \qquad p_2 = q_2 + a, \qquad p_3 = q_3 - 2a,$$

where $a = \frac{1}{4}(q_3^2 - 4q_1q_2)$. Thus, $p_1 - p_2 = q_1 - q_2 = \rho$, say. These results, together with (21), give

$$p_1 = \frac{1}{4}(1+\rho)^2, \qquad p_2 = \frac{1}{4}(1-\rho)^2, \qquad p_3 = \frac{1}{2}(1-\rho^2)$$

showing that ρ uniquely determines a point on the equilibrium parabola. Contours of constant ρ are linear, being given by the intersection of the planes $\mathbf{1}'\mathbf{q} = 1$ and $q_1 - q_2 = \rho$. These contours are shown on the left-hand side of Fig. 1 where they may be compared with the contours normal to the equilibrium parabola, given by least squares.

Because the multinomial estimates are so easily calculated, the least-squares solution may be thought redundant both on statistical and computational grounds. Yet the example has pedagogical interest (see Fig. 1) both in comparing different estimators and in the handling of constraints. Furthermore, the discontinuity in the first differential of the multinomial contours is worth noting.

2.6. Regression with an indefinite constraint

Cases where $\mathbf{B}$ is indefinite are uncommon but do exist in the literature. Thus, Gower and Dijksterhuis [12] require $\mathbf{x}'\mathbf{B}\mathbf{x} = -1$, where $\mathbf{B}$ is the Householder transformation $\mathbf{I} - 2\mathbf{ee}'$ where $\mathbf{e}$ is a zero vector apart from a single unit value.

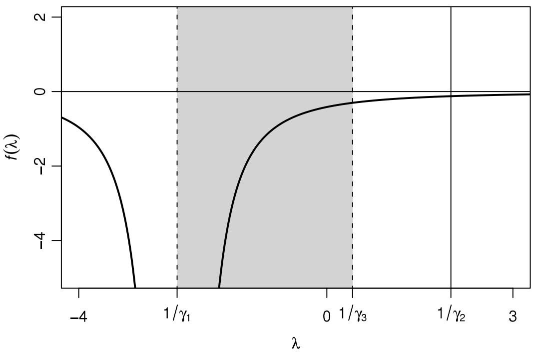

Fig. 2. Lagrangian $f(\lambda)$ for the example in Section 2.6 with zero values of s_i. There are phantom asymptotes at $1/\gamma_2$ and at $1/\gamma_3$, the upper bound of the admissible region, so the minimum occurs at $\lambda = 1/\gamma_3$.

In this section, we outline a problem with its origins in the ALSCAL algorithm. ALSCAL [24] is a well-known alternating least-squares multidimensional scaling algorithm for minimising the metric SSTRESS criterion $\sum_{i<j}(d_{ij}^2 - \delta_{ij}^2)^2$ where d_{ij} are observed distance-like quantities and δ_{ij} are Euclidean distances generated by points in some small number of dimensions, whose coordinates are required. Ten Berge [25] has noted that the algorithm requires the solution to a constrained regression problem and gave a bespoke solution. In our notation, Ten Berge's specification requires

$$\left.\begin{array}{l} \min_{\mathbf{x}} ||\mathbf{d} - \mathbf{K}\mathbf{x}||^2 \\ \text{subject to } x_2^2 = 4x_1x_3 \end{array}\right\}$$

where

$$\mathbf{d} = \begin{pmatrix} 0.6533 \\ 0.2706 \\ 0.2706 \\ 0.6533 \end{pmatrix} \quad \text{and} \quad \mathbf{K} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 2 & 4 \\ 1 & 2 & 4 \\ 1 & 3 & 9 \end{pmatrix}.$$

The indefinite constraint looks like (19) but, not being subject to further conditions of Hardy–Weinberg, cannot be reduced to the two-dimensional parabolic form discussed in Section 2.5. We may write the objective function in the form (1) as follows:

$$\min_{\mathbf{x}} ||\mathbf{d} - \mathbf{K}\mathbf{x}||^2 = \min_{\mathbf{x}}(\mathbf{x} - \mathbf{t})'\mathbf{A}(\mathbf{x} - \mathbf{t}) + \text{constant},$$

where $\mathbf{A} = \mathbf{K}'\mathbf{K}$ and $\mathbf{t} = (\mathbf{K}'\mathbf{K})^{-1}\mathbf{K}'\mathbf{d}$. The matrix form of the constraint is

$$\mathbf{x}'\mathbf{B}\mathbf{x} = \mathbf{x}' \begin{pmatrix} & & -2 \\ & 1 & \\ -2 & & \end{pmatrix} \mathbf{x} = 0,$$

where $\mathbf{B}$ has eigenvalues $(-2, 1, 2)$, confirming that $\mathbf{B}$ is indefinite. Both $\mathbf{A}$ and $\mathbf{B}$ are of full rank permitting the GCF to simplify to $\mathbf{T}'\mathbf{B}\mathbf{T} = \text{diag}(\mathbf{\Gamma}_1) = (1 - \sqrt{2}, 1/2, 1 + \sqrt{2})$ and $\mathbf{s} = \mathbf{T}\mathbf{t} = (0, 0, -1)$ on a principal axis of B. Asymptotes of the GCE are at $\lambda = 1/\gamma$ with values, in ascending order, of $\text{diag}(-(\sqrt{2} + 1), \sqrt{2} - 1, 2)$. The first two elements contain the origin and hence define the admissible region. Then the FCE $f(\lambda) = 0$ has two phantom asymptotes, one at the upper boundary of the admissible region, shown shaded in Fig. 2. The optimal λ is given by the boundary of the admissible region at $\lambda = 1/\gamma_3 = \sqrt{2} - 1$. Then, $\mathbf{z}$ is computed according to Section 3.1 on zero values of s_i of Albers et al. [2], yielding two simply related solutions $\mathbf{z} = \left(-\frac{1}{4}(2 + \sqrt{2}), 0, \pm 8^{-1/2}\right)' = (-0.8536, 0, \pm 0.3528)'$. The original parameters are given by $\mathbf{x} = \mathbf{T}^{-1}\mathbf{z} = (2.6132, -2.6132, 0.6533)'$ and $\mathbf{x} = (0.467, 0, 0)'$, both giving the same minimum, in agreement with Ten Berge [25]. Although the two solutions for $\mathbf{z}$ differ only in sign, after transformation to $\mathbf{x}$ they have quite different appearances. For further discussion, see [1].

3. Conclusion

Our approach has two advantages.

First, the General Canonical Form (2) transforms the minimisation problem (1) into a much simpler problem, much in the same way as do the canonical forms arising from the classical algebraic eigenvalue problem. Many problems, when expressed in terms of the general canonical variables, reveal structure that illuminates understanding (see e.g. Sections 2.1, 2.6 and 2.5). This in itself is valuable.

Second, the minimisation of the GCF of (1) is amenable to detailed analysis which shows that there is a unique minimum calculable by a well-defined algorithm that handles all cases. This does not mean that the general algorithm will be faster than tailor made algorithms for the problems we have discussed, and others like them. However, the computational efficiency of a tailor made algorithm may be totally outweighed by the inefficient use of human time taken in its development, much will depend on how often the algorithm is used. In any case, it is useful to have the general algorithm that takes cognisance of all the pitfalls revealed by our analysis (phantom asymptotes interplay of null and range spaces, problems with indefinite and semi-definiteness, zero k) to act as a yardstick when developing tailor made software.

We hope that this paper has demonstrated the generality and utility to statisticians of the minimisation problem (1). Although not so fundamental as the algebraic eigenvalue problem, on which part it depends, it is a useful addition to the tools available to researchers.

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